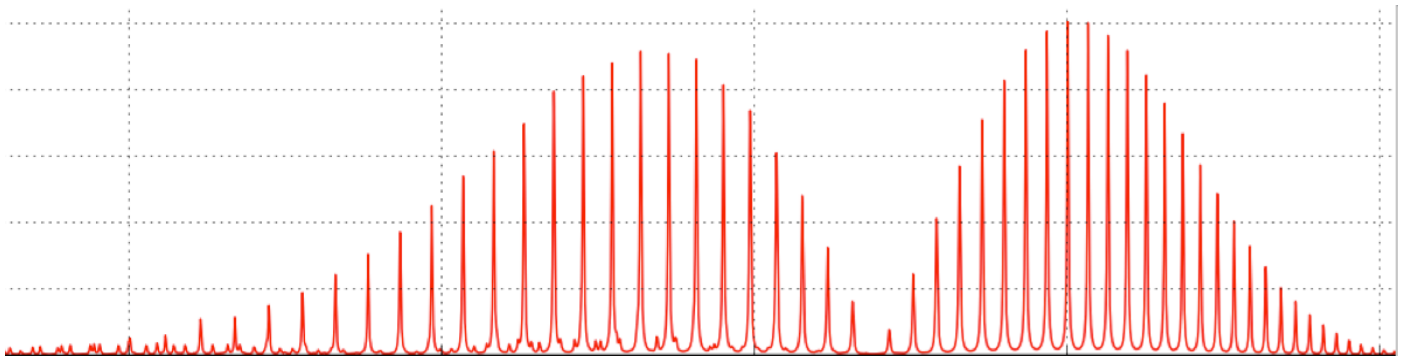
ABSCO status and plans

Vivienne Payne, Jet Propulsion Laboratory, California Institute of Technology

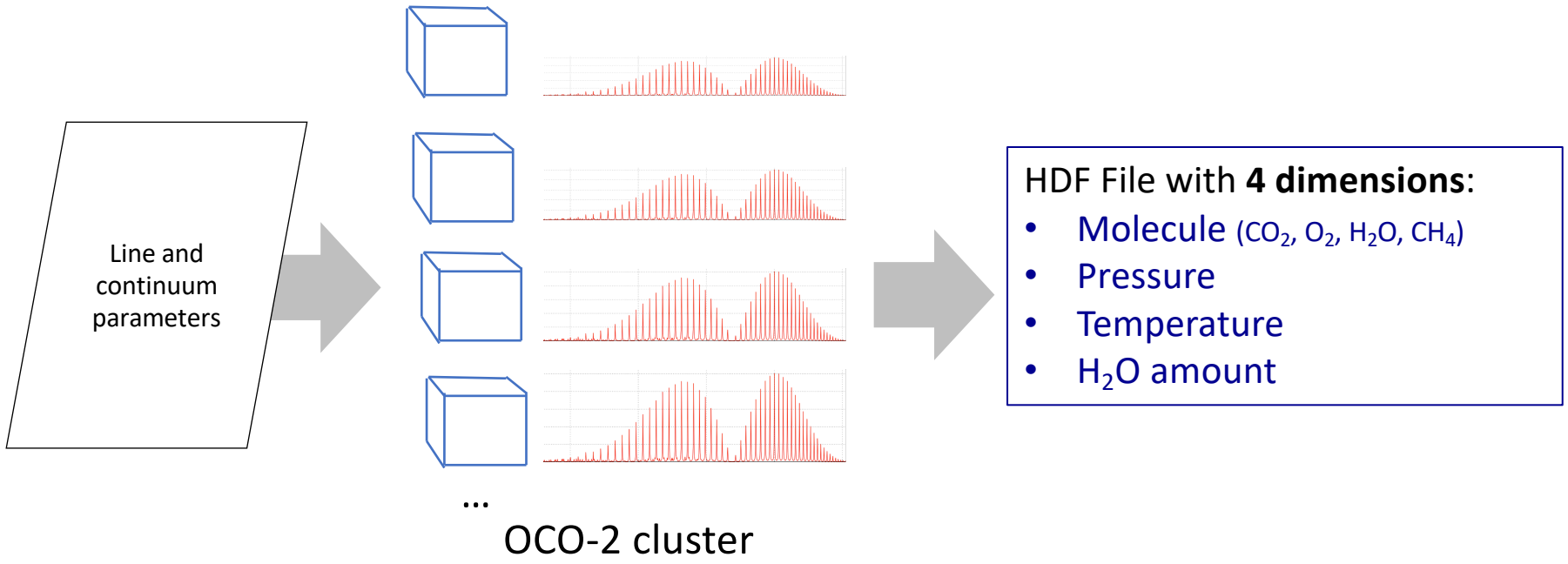
On behalf of the OCO-2 ABSCO team



Absorption coefficient (ABSCO) tables

ABSCO version	L2 version
v4.2	B7
v5.0	B8
v5.0	B9
v5.1	**B10**

- Problem: Advanced spectroscopic models too slow for online use
- Solution: pre-computed lookup table for linear interpolation
- Compute cross sections at independent temperatures, pressures, H_2O amounts



Evaluation of absorption coefficients

Image: JAXA

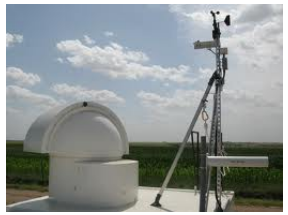


Image: Caltech

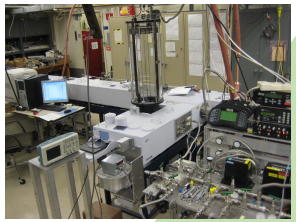


Image: JPL

Satellite soundings

- 1-3 bands, multiple absorbers
- Low spectral resolution
- **Full atmospheric path**
- Unconstrained atmosphere, aerosols, surface albedo

TCCON spectra

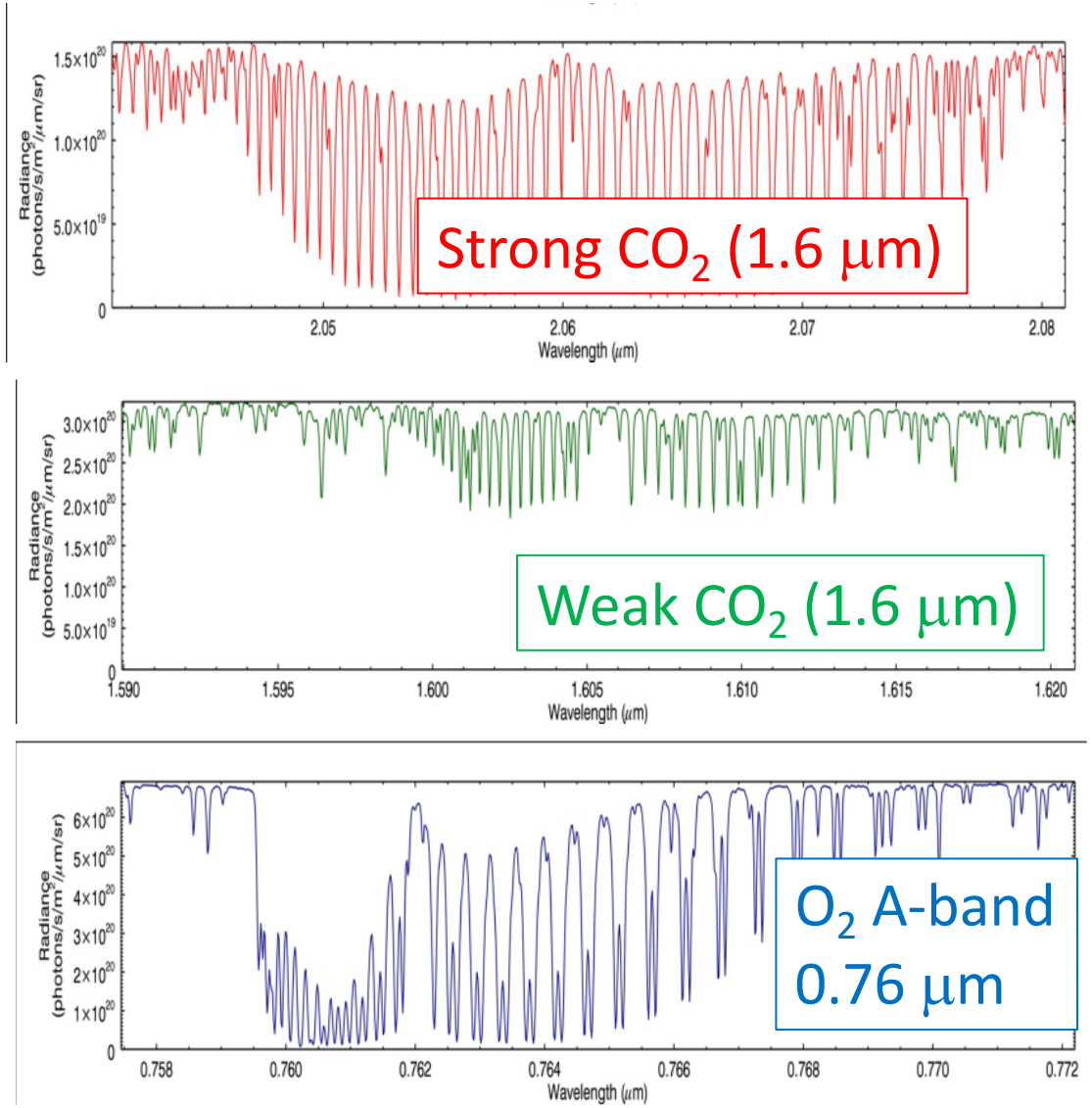
- 1-3 bands, multiple absorbers
- High spectral resolution
- **Full atmospheric path**
- Constraints on atmospheric conditions

Laboratory spectra

- 1 band, one absorber
- High spectral resolution
- Known laboratory conditions

Overview

- ABSCO v5.1
  - ABSCO version for B10 Level 2 algorithm
  - What's new compared to ABSCO v5.0
- Beyond ABSCO v5.1
  - Improvements under development for the next ABSCO update and beyond



What's new: Spectroscopic updates for ABSCO v5.1

- H_2O: Updated continuum
  - Leads to reduction in H_2O dependence of surface pressure bias
- O_2 updates (**delivered in October 2018**)
  - Reduction in chi^2 values
  - Flattening of latitudinal gradients in the surface pressure bias.
- CO_2 unchanged from 5.0
- ABSCO v5.1 has been adopted for the B10 L2 algorithm

Details: CO_2 bands

ABSCO Tables		V5.0	V5.1
4850 cm^{-1} CO_2 20013 -> 00001	**Line shape**	Speed Dependent Voigt, fit to range of temperatures **[Benner et al., 2016]**	Speed Dependent Voigt, fit to range of temperatures **[Benner et al., 2016]**
	Line mixing	Nearest-neighbor from multi-spectrum fit [Benner et al., 2016]	Nearest-neighbor from multi-spectrum fit [Benner et al., 2016]
	Ad-hoc absorption	Ad hoc	Ad hoc
	H_2O-CO_2 broadening	Sung et al. [2009]	Sung et al. [2009]
6220 cm^{-1} CO_2 30013->00001	**Line shape**	Speed Dependent Voigt fit to range of temperatures **[Devi et al., 2016]**	Speed Dependent Voigt fit to range of temperatures **[Devi et al., 2016]**
	Line mixing	Nearest-neighbor from multi-spectrum fit **[Devi et al., 2016]**	Nearest-neighbor from multi-spectrum fit **[Devi et al., 2016]**
	H_2O-CO_2 broadening	Sung et al. [2009]	Sung et al. [2009]
H_2O and CH_4 in CO_2 bands	**H_2O continuum**	Supplied by E. Mlawer	**MT_CKD v3.2**
	H_2O lines	HITRAN 2012	**HITRAN 2012**
	CH_4 lines	Not included	Not included

Scaling of absorption coefficients applied within L2 code.
Scale factor: 1.004

ABSCO tables supplied pre-scaled, with scaling factor (1.014) based on difference between Devi et al. and NIST reference intensities for a few strong lines

Details: CO_2 bands

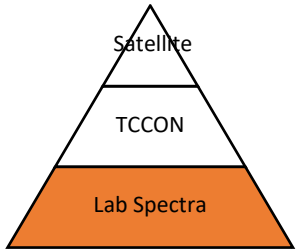
- Notes:
  - **There is still <u>plenty</u> of room for improvement in modeling of CO_2 lineshape/line mixing!**
  - **H_2O spectroscopy also an important consideration**
    - H_2O continuum impacts OCO-2 PSUR retrieval via impact of SCO2 on PSUR
      - Future continuum updates under consideration at AER, in light of new CRDS measurements from Campargue group
    - H_2O line parameters impact OCO-2 XCO_2 for high-H_2O regions
      - No H_2O line parameter update for ABSCO v5.1
      - Future updates under discussion, pending input from I. Gordon et al.

Details: O_2 A-band

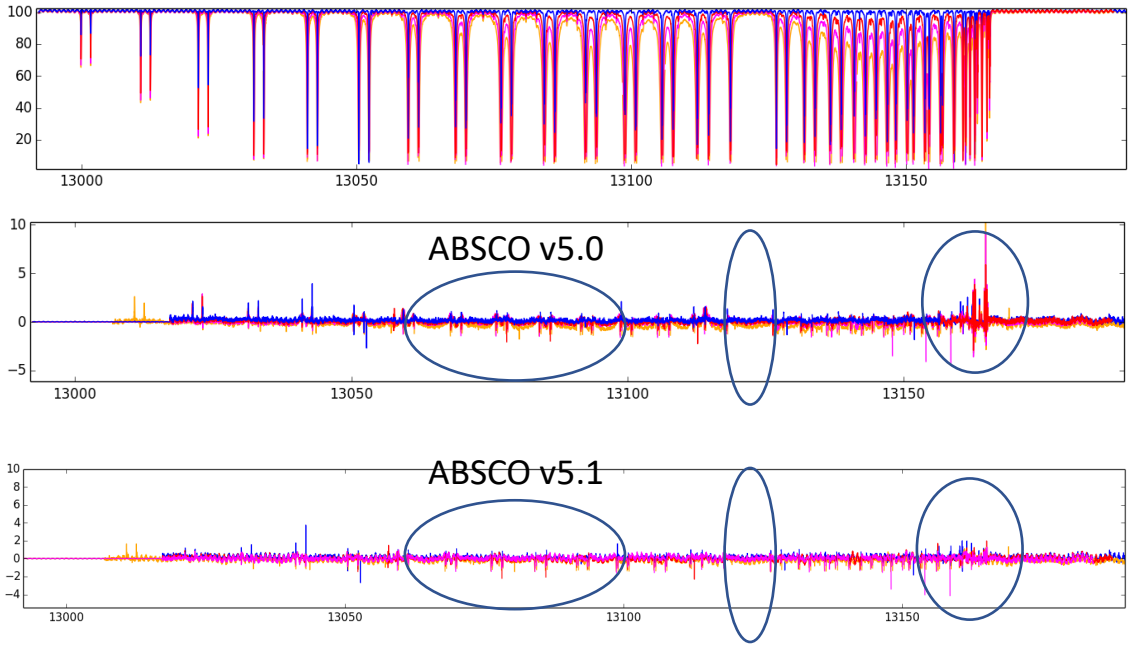
ABSCO Tables		v5.0 (L2 B8, B9)	v5.1 (L2 B10)
13200cm^{-1} O_2	**Line shape**	Speed-dependent Voigt (SDV) from self-consistent set of multi-spectrum fits, utilizing FTS and CRDS measurements **(Drouin et al. 2017)**	SDV from self-consistent set of multi-spectrum fits, utilizing FTS and **additional CRDS** measurements **T-dependent foreign parameters from CRDS**
	Line mixing	ΔJ = even / sub-bands	**Include ΔJ = odd / inter-band for O_2-N_2**
	Collision Induced Absorption (CIA)	From ground-based atmospheric measurements at Lamont (E. Mlawer, AER) and CRDS	From ground-based atmospheric measurements at Lamont (E. Mlawer, AER), **updated for consistency with line parameter and line mixing updates**
	H_2O-O_2 broadening	Drouin et al. [2014]	Drouin et al. [2014]

O_2 A-band spectroscopy update

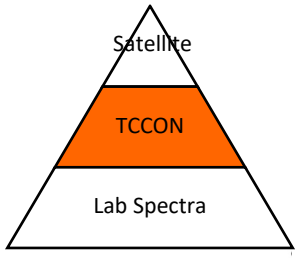
New multispectrum fits for O_2:
Laboratory residuals from NIST CRDS

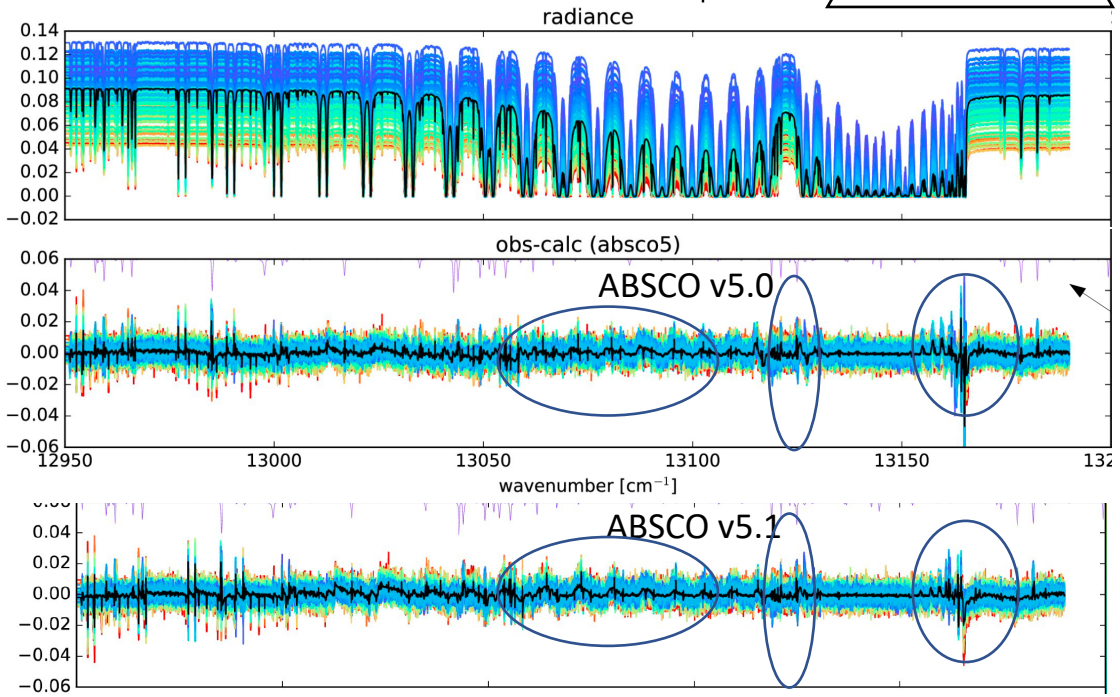


290 K, 2.0% O_2, 100-1000 Torr



Evaluation with Lamont TCCON spectra





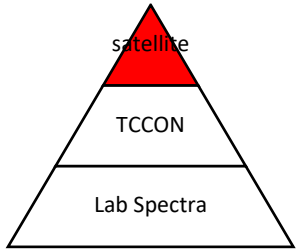
Solar lines

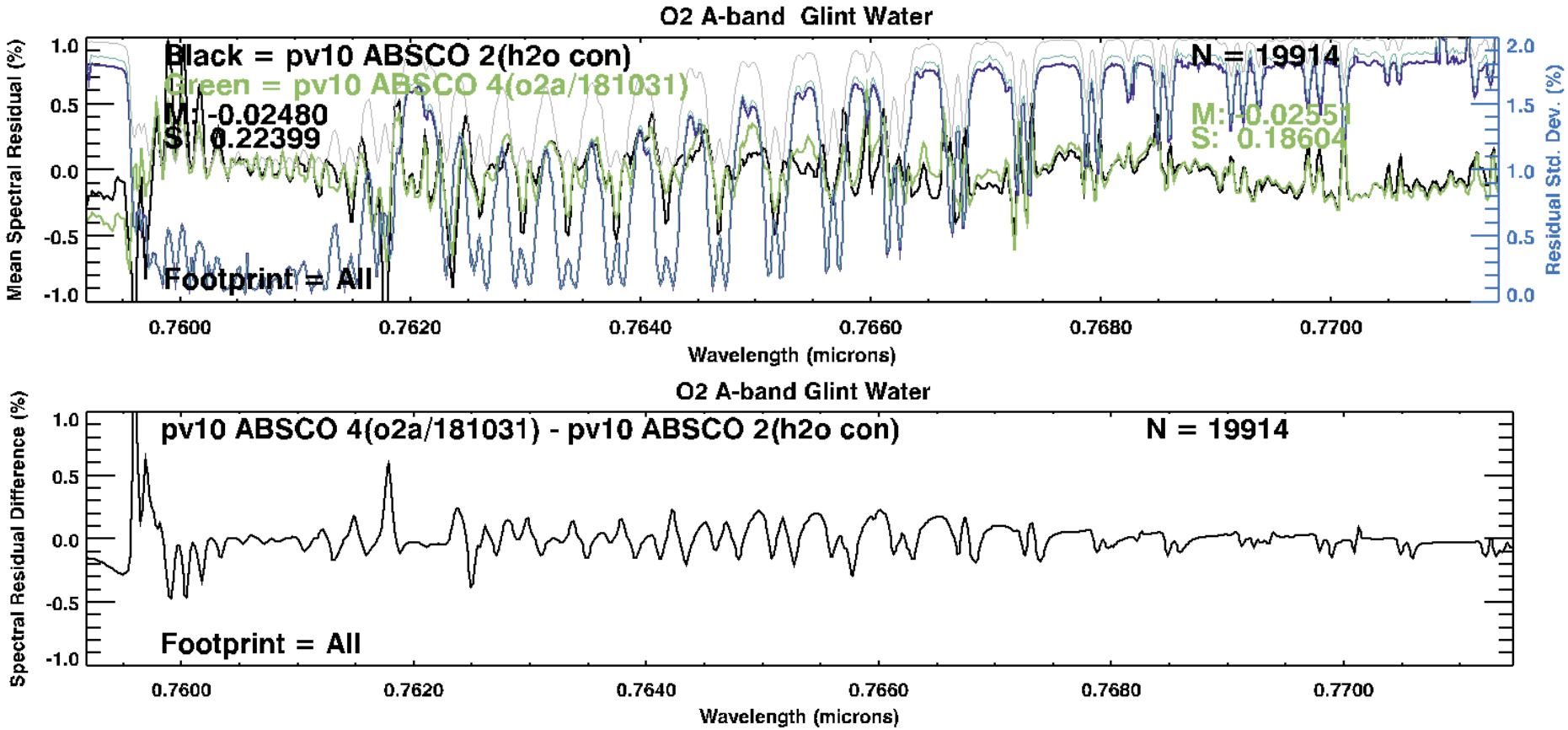
Improvements:
At R branch bandhead
Between P&R branches

Lab figures: B. Drouin

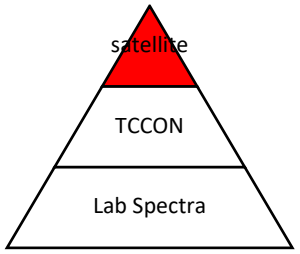
TCCON residual figures: F. Oyafuso

O_2 update: “No-EOF” Residuals

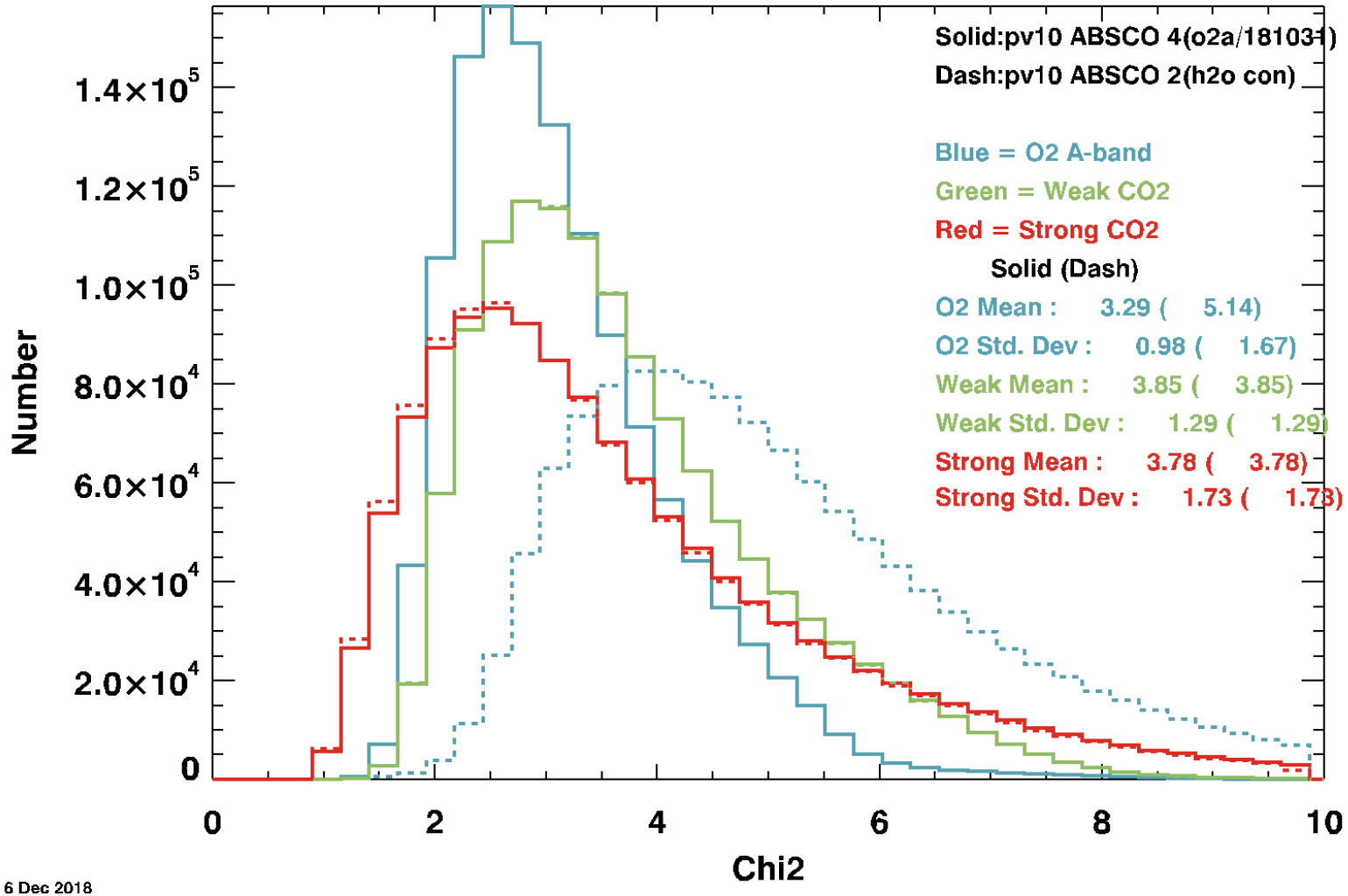




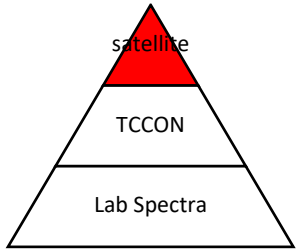
Significant differences (improvement) in the OCO-2 “no-EOF” spectral residuals



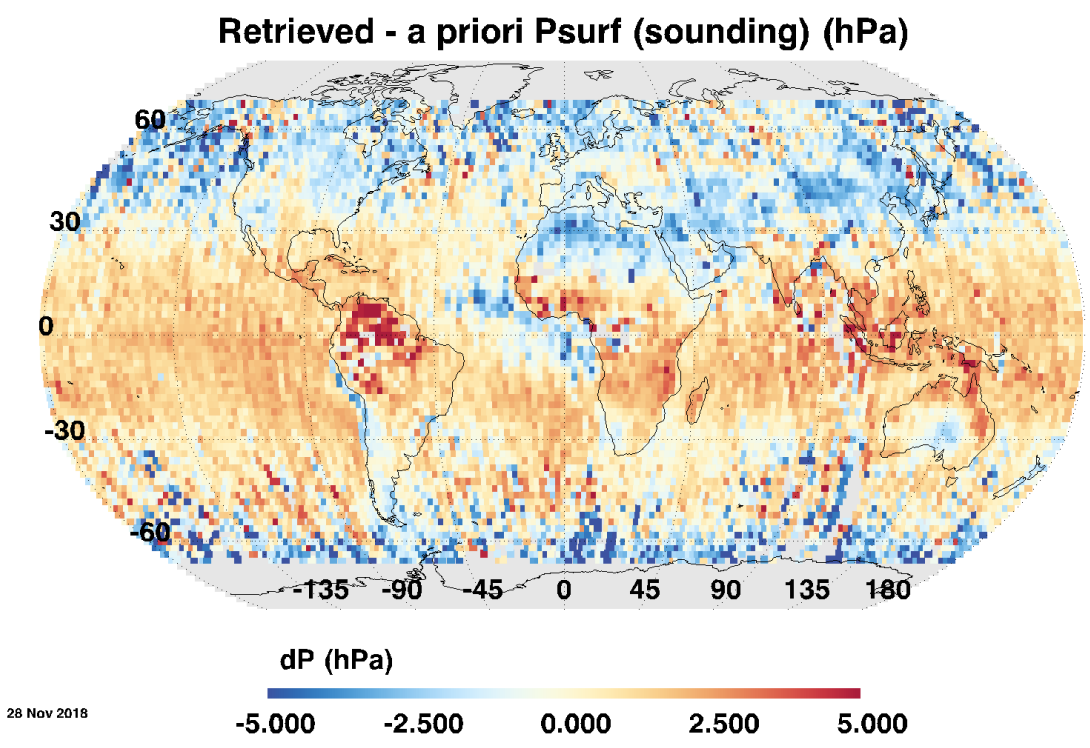
O_2 update results in significant reduction in chi-squared



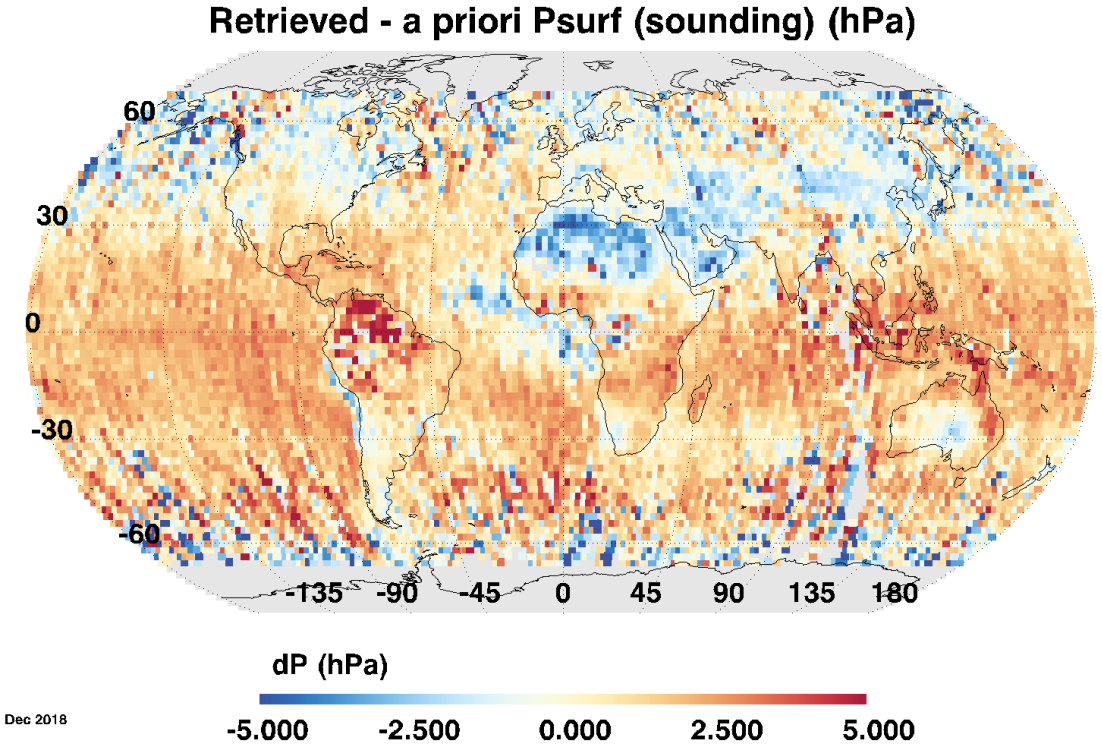
O_2 update: Retrieved – prior Psurf
”No-EOF” results



Before O_2 A-band update



After O_2 A-band update



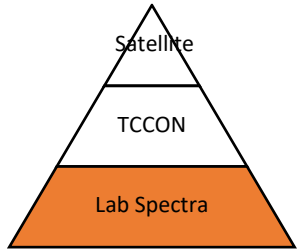
Satellite test sets used for evaluation of this ABSCO update are much more extensive than those used in evaluation of ABSCO v5.0

Figures: B. Fisher

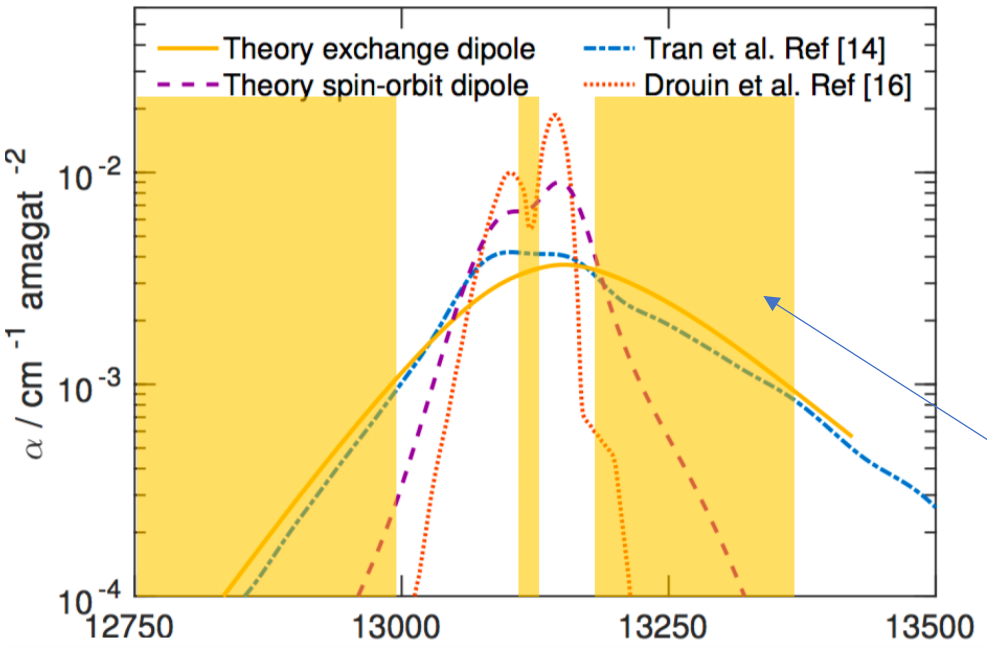
September 2019 ABSCO delivery (and beyond)

- O_2
  - Inclusion of new and re-calibrated CRDS spectra, after addressing digitizer non-linearity (NIST)
  - Harnessing PAS spectra to assess model consistency, inform quantitative analysis (Caltech)
  - Inclusion of information from new high pressure FTS measurements (JPL)
  - **Laboratory constraints on collision-induced absorption**
  - **Re-evaluation of line mixing formulation**
  - Include H_2O-O_2 broadening in collision-induced absorption?
- CO_2
  - Going beyond nearest-neighbor **line mixing**, to remove ad-hoc SCO_2 absorption
  - Revisit fitting of WCO_2, constrained by intensities from available NIST CRDS measurements
  - **Revisit fitting of** SCO_2, band constrained by NIST intensities (measurements underway at NIST)
- H_2O
  - Updates to **self- and foreign-broadened MT_CKD continua** in SCO2 and WCO2
    - based on new measurements from Alain Campargue's group
  - Re-visit **water vapor line parameters in SCO2, WCO2 and O2 A-band**
    - based on advice from I. Gordon, E. Conway
  - Include info from targeted NIST H_2O line measurements

O_2 A-band: Collision-induced absorption

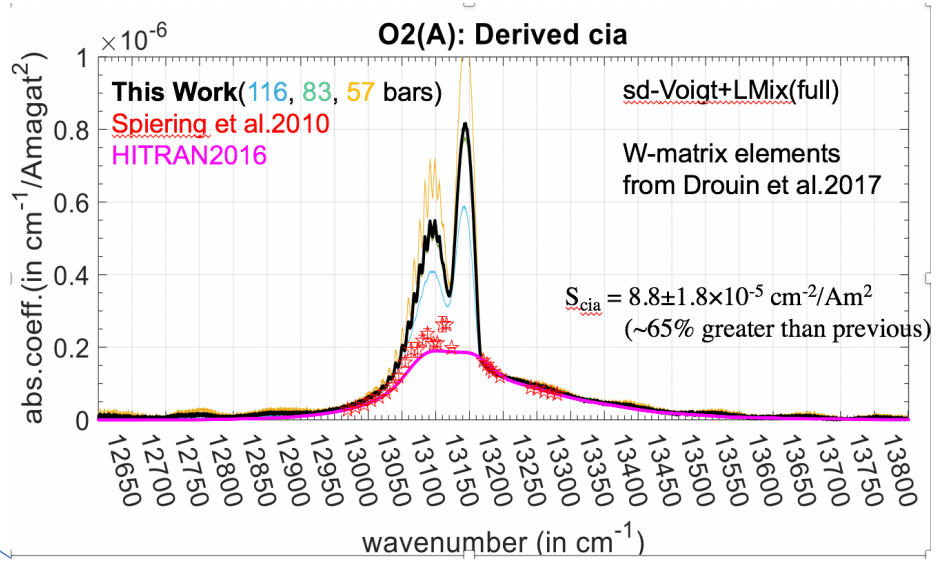


New developments in theory



Tijs Karman, Collision-induced absorption by oxygen and nitrogen molecules.
Raboud University, 2018

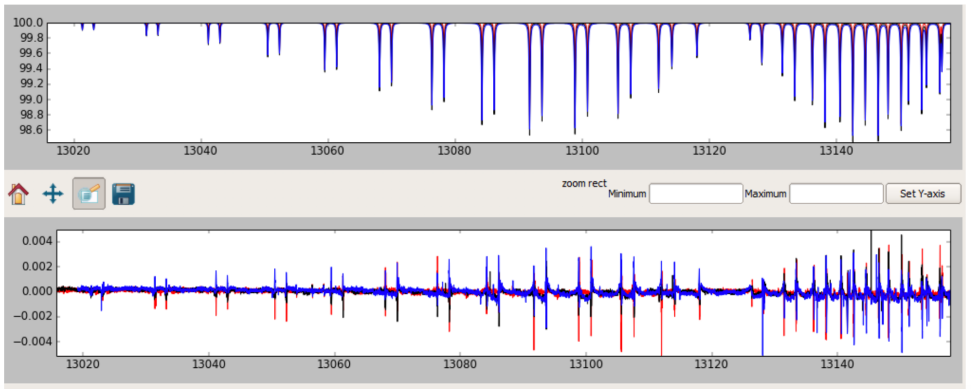
Multi-pronged effort on laboratory constraints on CIA



High-pressure FTS measurements completed
(K. Sung, JPL)

CRDS measurements being made in shaded regions (E. Adkins, NIST)

Improved PAS measurements underway
(E. Lunny, Caltech)



CO_2 line mixing: Revisit existing FTS lab spectra

Examine most sensitive data, ran multispectral fit with LM changed/floated near diagonal, full and partial cross-band coupling

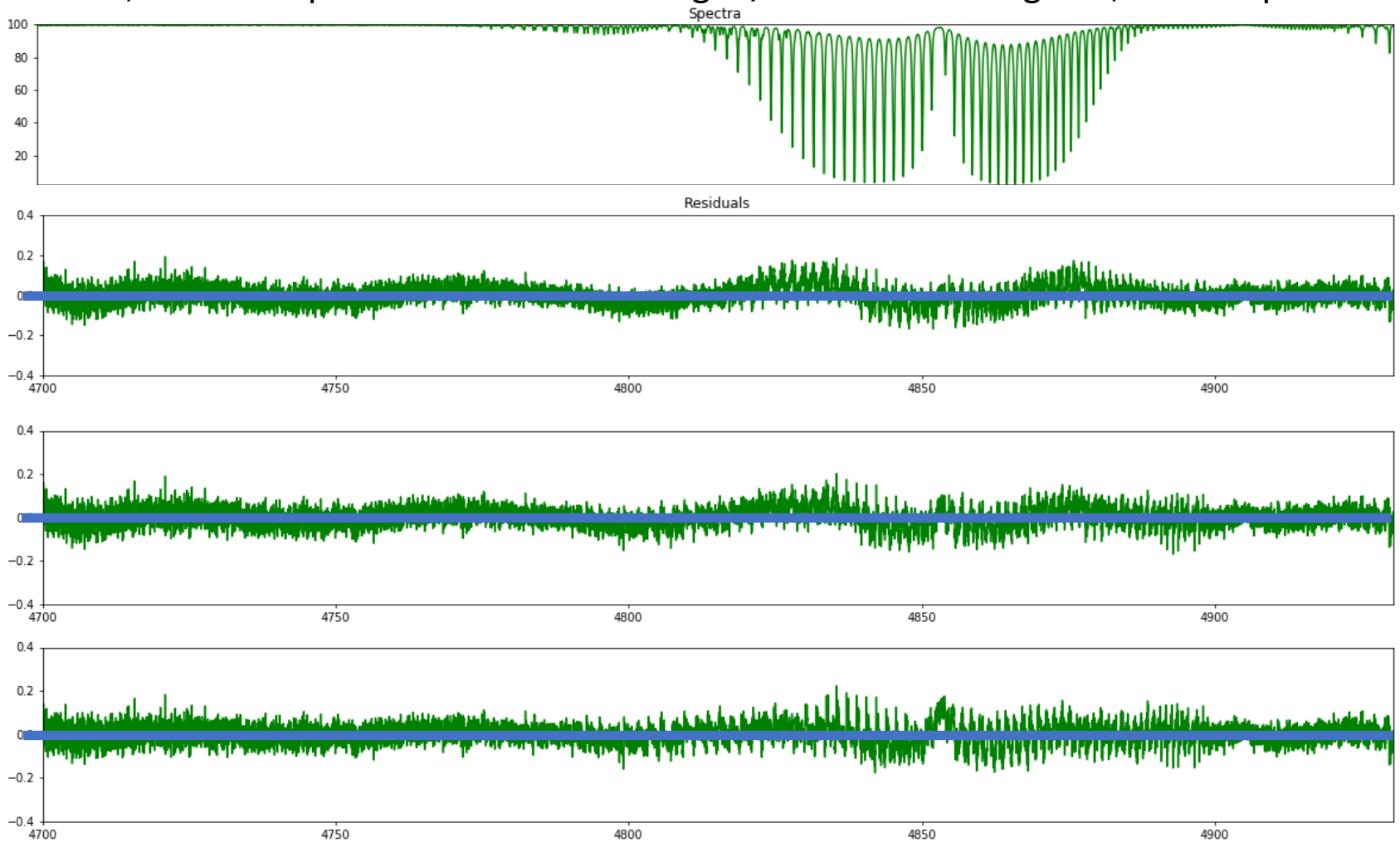
Spectrum
3809

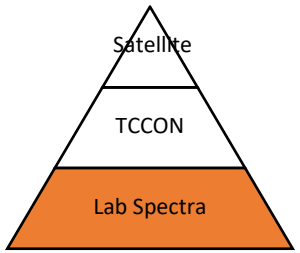
Devi*
44.6 overall
45.0 3809

Lamouroux

LM RPx0.5
44.7 overall
43.8 3809

LM RPx1
45.0 overall
45.8 3809

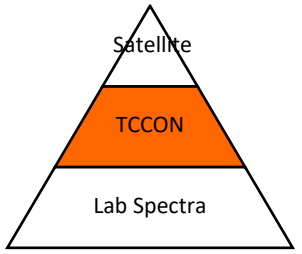


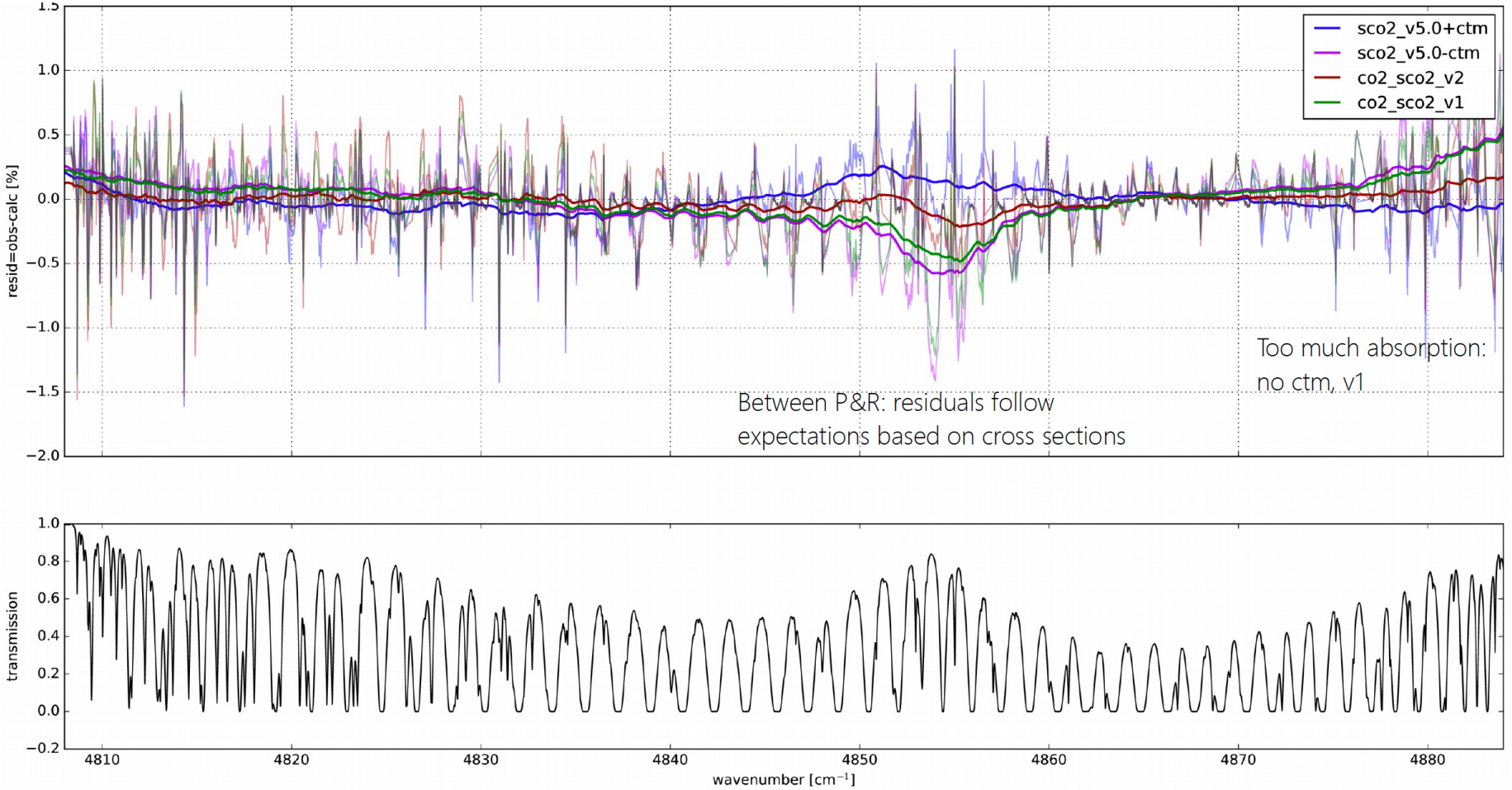


20.8778 m, -52.95 °C, 650 Torr, 5% CO2, 95% air

Brian Drouin

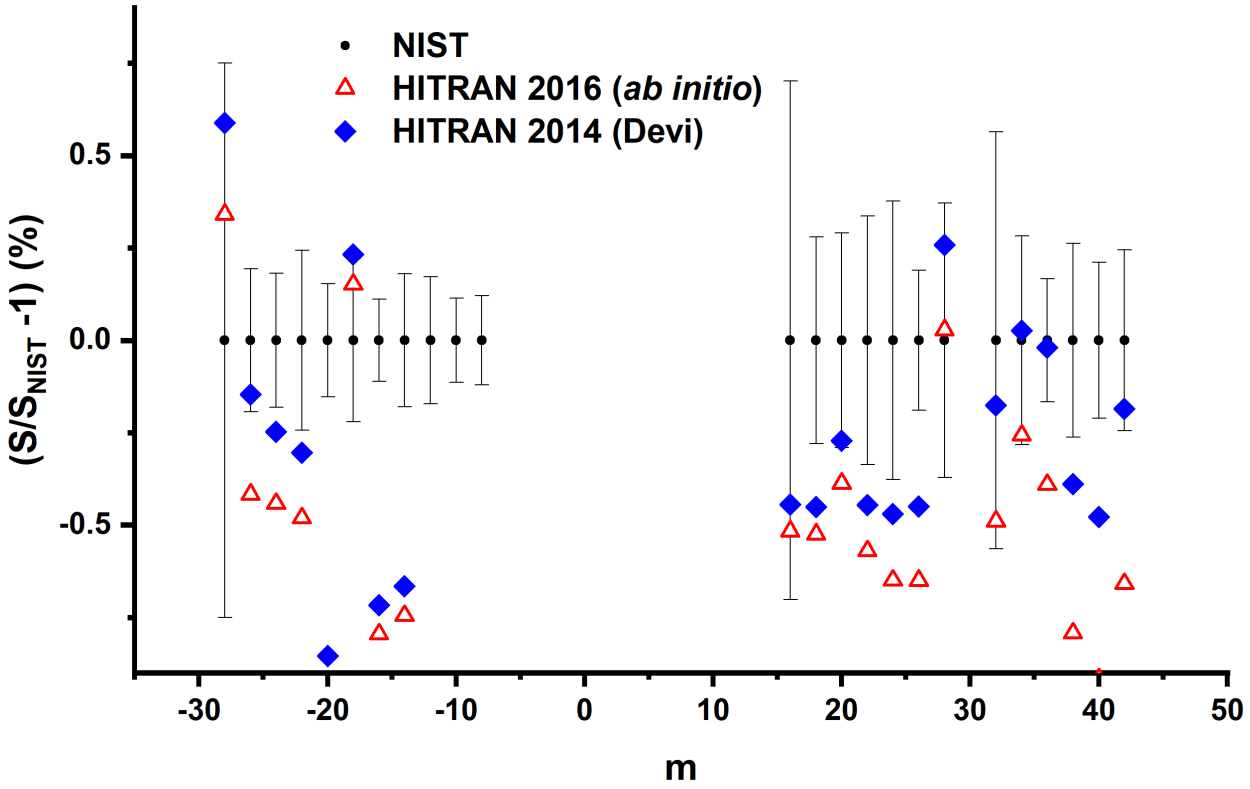
SCO_2 line mixing: Evaluation with TCCON spectra





Fabiano Oyafuso

Preliminary results for OCO strong band



0.37 % average difference relative to Devi (HITRAN 2012)

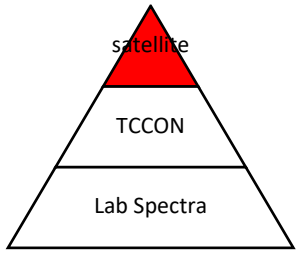
Next Steps

Now setting up new ECDL to span the wave number range 4820 cm^{-1} to > 5000 cm^{-1} where we will repeat intensities and extend J-range, and take continuous spectra at elevated pressures (up to 1000 Torr), to quantify line mixing effects.

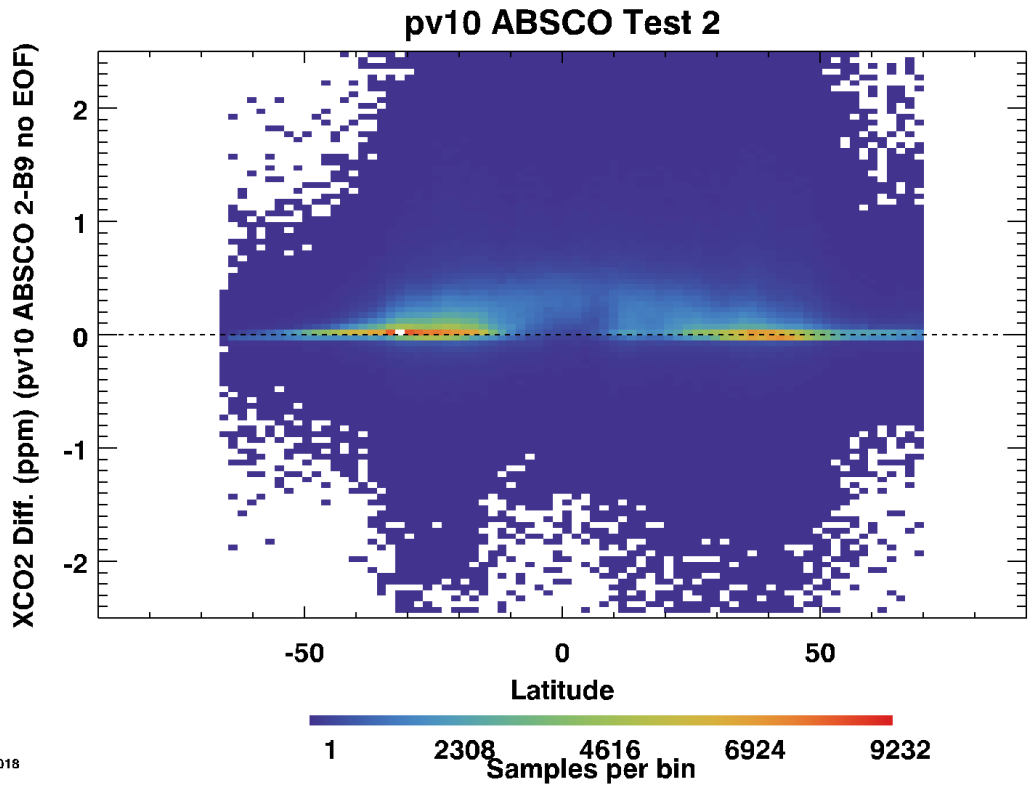
We will also measure H_2O interferences.

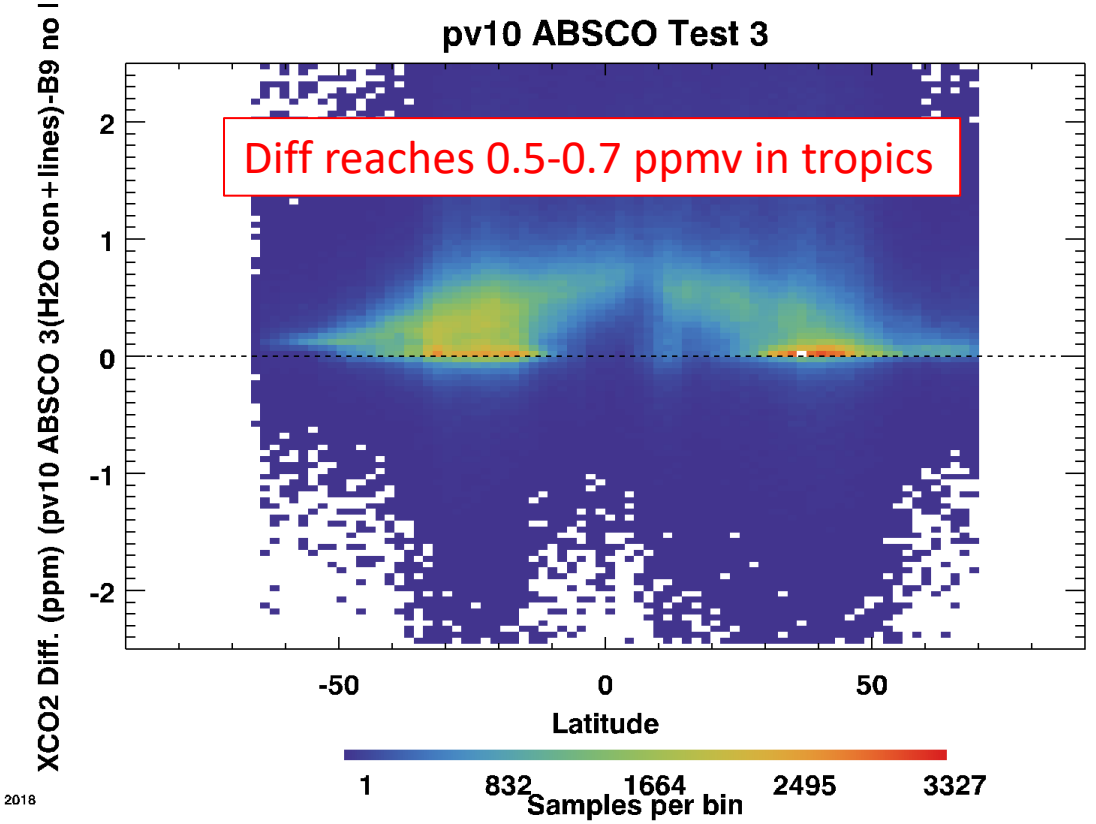
J. Hodges et al.

Impact of changing H_2O line parameter database



Difference between these two plots is the difference between using HITRAN 2012 vs HITRAN 2016 H_2O





Test 2: Impact of H2O continuum update on XCO2

Test 3: Impact of H2O continuum **+ lines** update on XCO2

Figures: B. Fisher

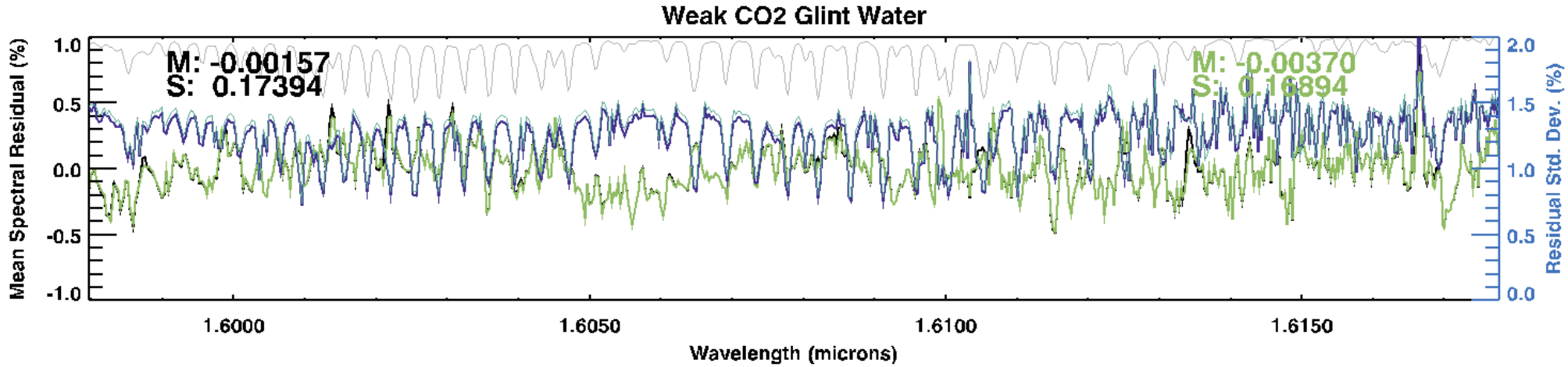
For regional biases, H_2O spectroscopy is an important consideration!

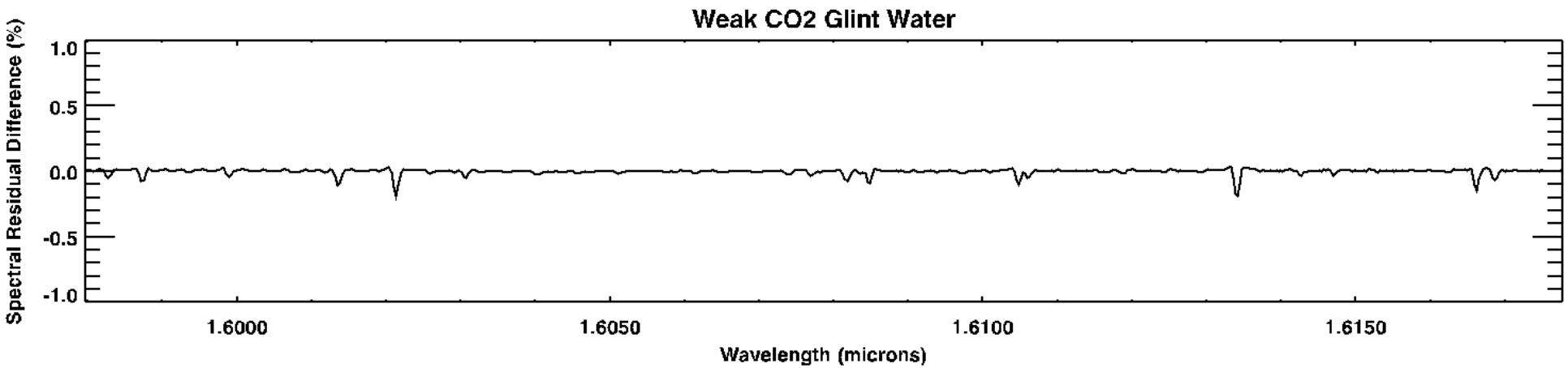
2019 ABSCO timeline

- Spring
  - New high-pressure laboratory FTS measurements for O2 A-band
  - Re-evaluate 2.06 micron line mixing based on currently available measurements
  - Design of approach for evaluation of ABSCO v5.1 uncertainties for updated linear error analysis
  - OCO-2/OCO-3 STM
- Summer
  - Expansion of TCCON test datasets
  - O2 A-band multispectrum fit analysis that includes new laboratory measurements
  - Evaluation of H_2O continuum updates
- August
  - Delivery of new lab-based analysis for O2 and CO2, plus updates to H2O line list and continuum
  - Creation of ABSCO tables (including completion of “perturbed” tables for linear error analysis)
  - Validation against atmospheric spectra
  - Evaluation of need for empirical adjustment to O2 A-band CIA, based on atmospheric results
- September
  - In-person meeting in Pasadena (week of 16th September)
  - Delivery of new ABSCO to L2 team
- October
  - OCO-2/OCO-3 STM, Colorado
  - Initial L2 testing results?

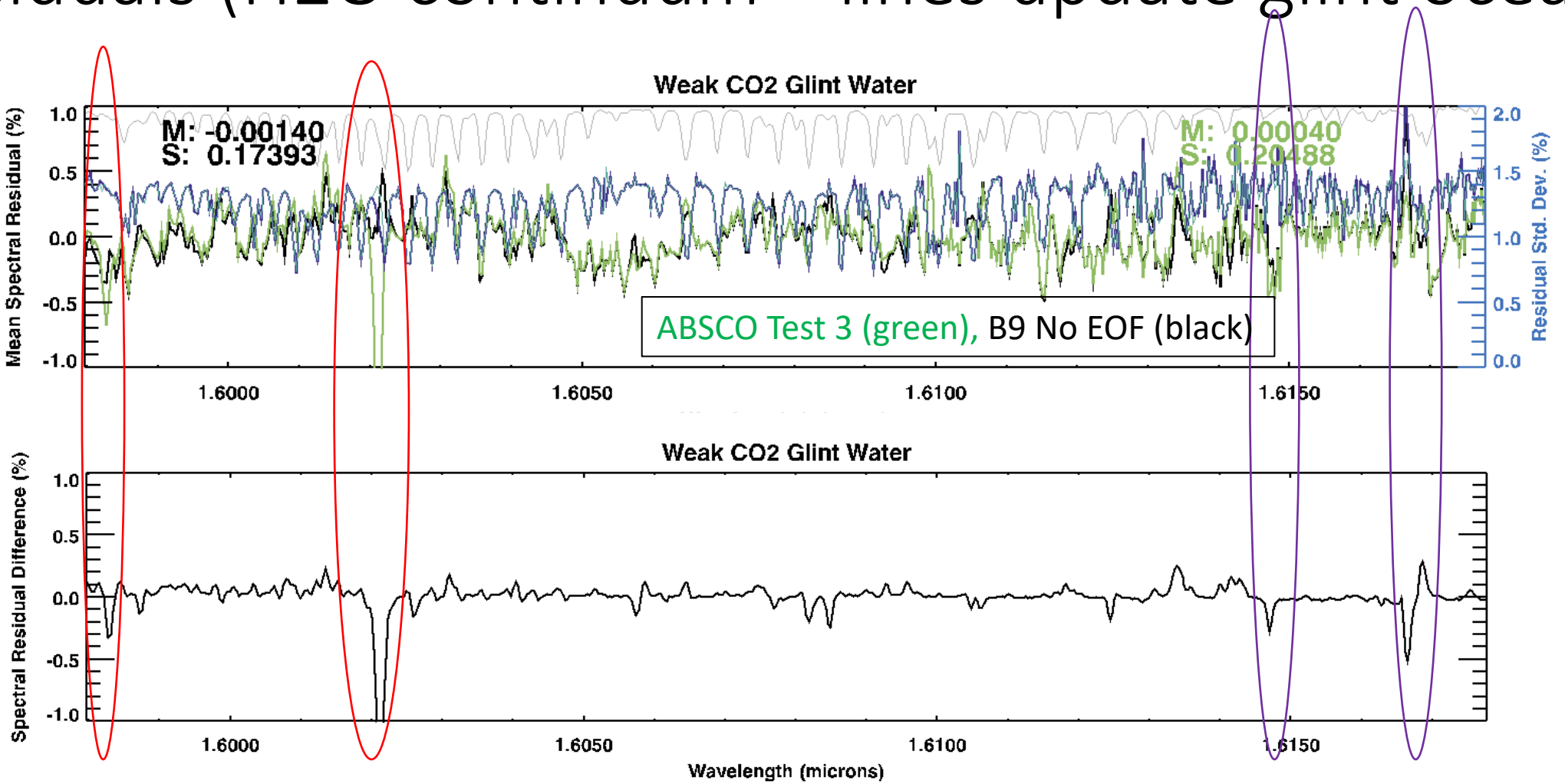
Backup slides

Residuals (H2O continuum update glint ocean)





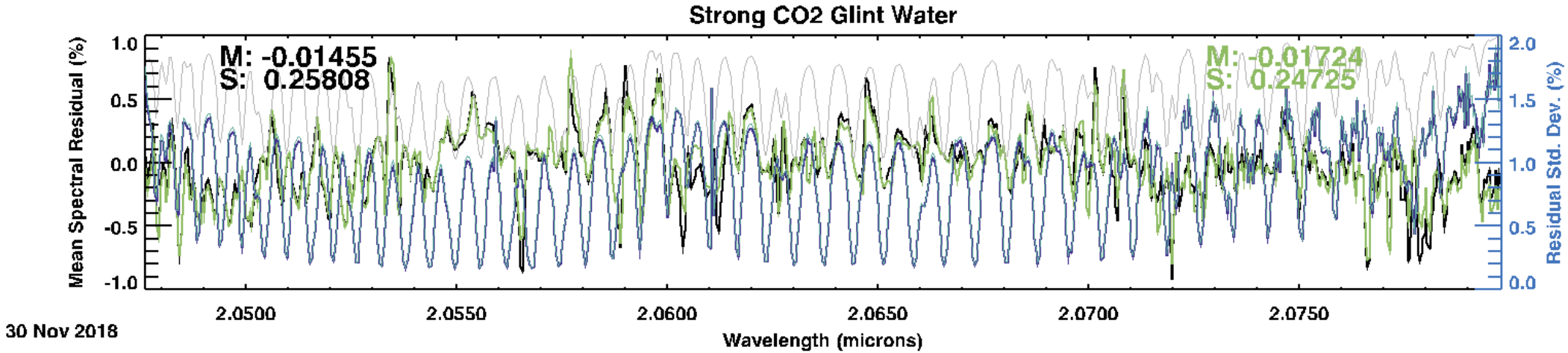
Residuals (H2O continuum + lines update glint ocean)

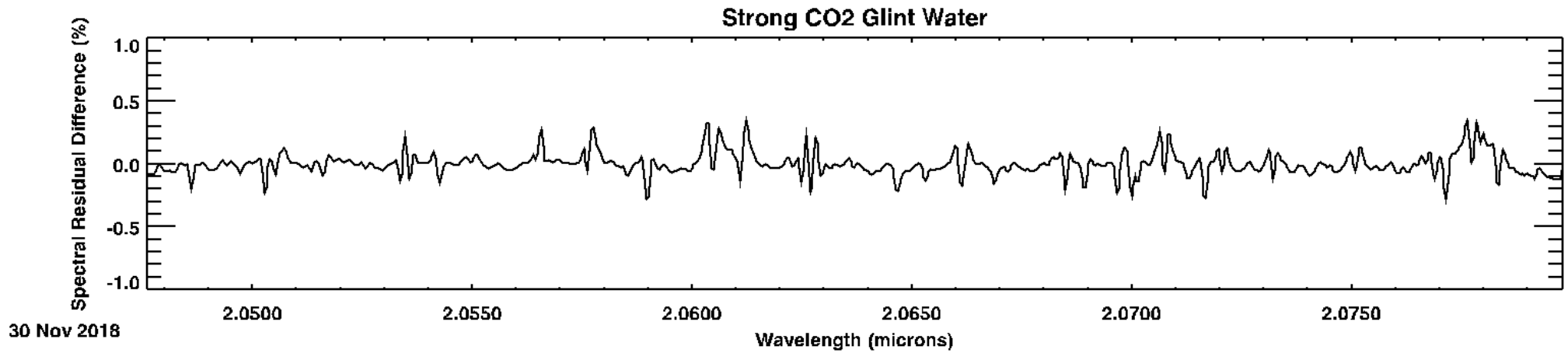


HITRAN 2016 “worse” than HITRAN 2012 in some places

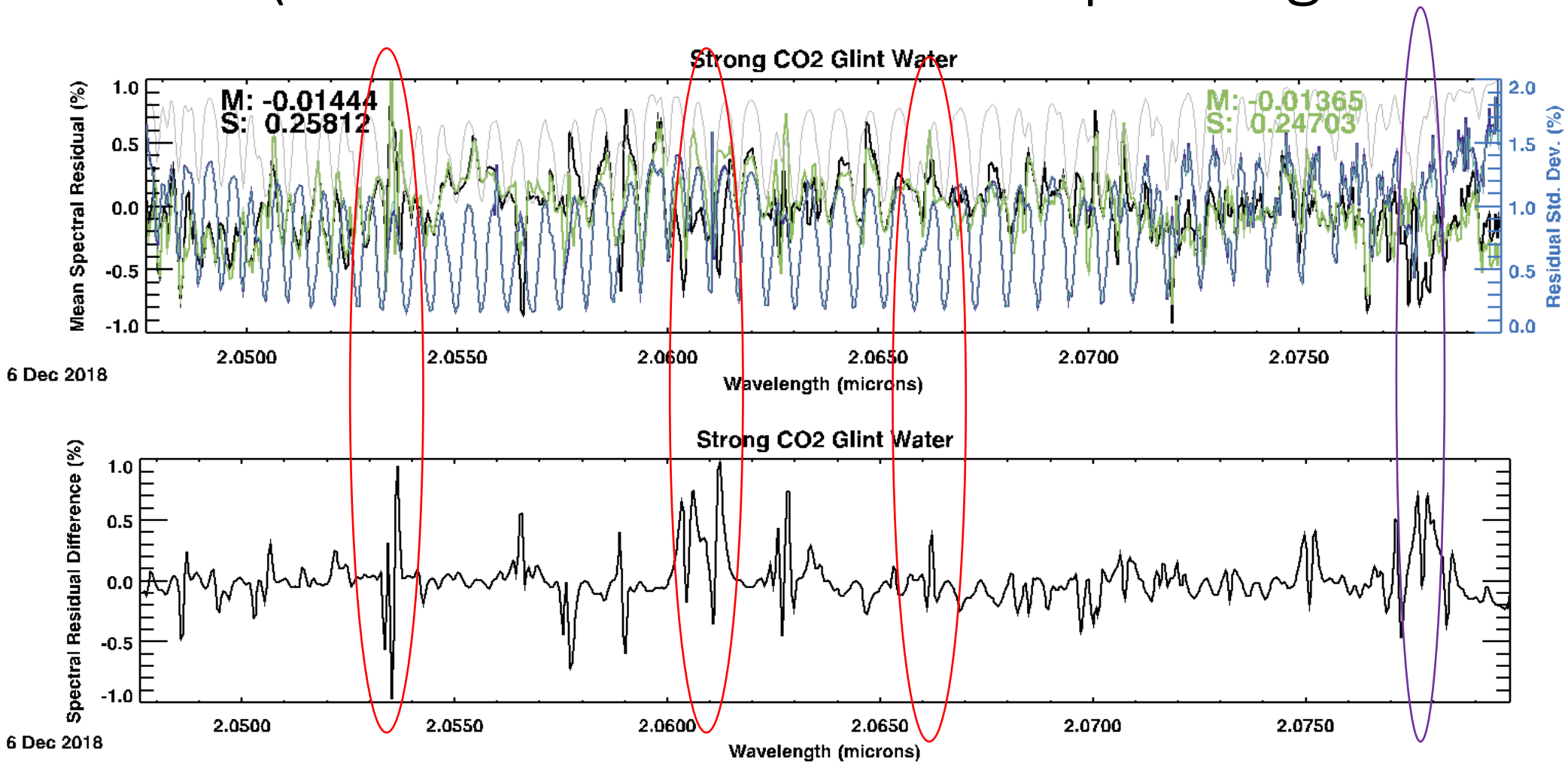
And “better” in other places….

Residuals (H2O continuum update glint ocean)



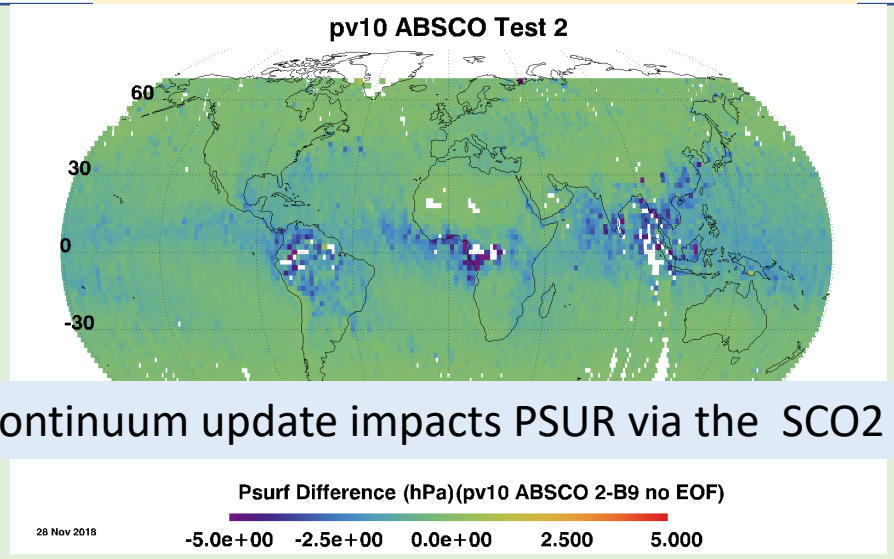


Residuals (H2O continuum + lines update glint ocean)

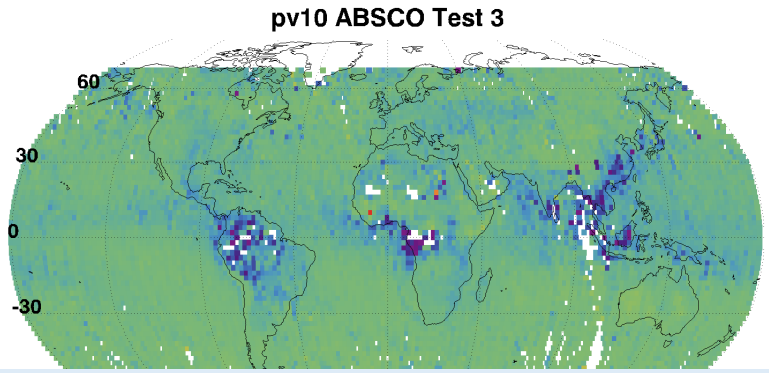


H_2O impacts (test 2=cntnm, test3=cntnm+lines)

Impact on retrieved surface pressure

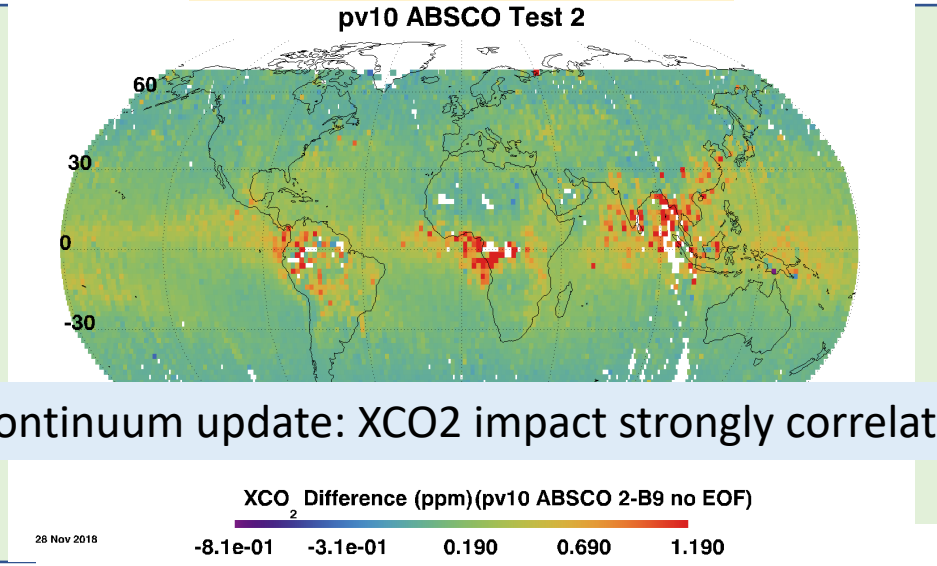


Continuum update impacts PSUR via the SCO2 band



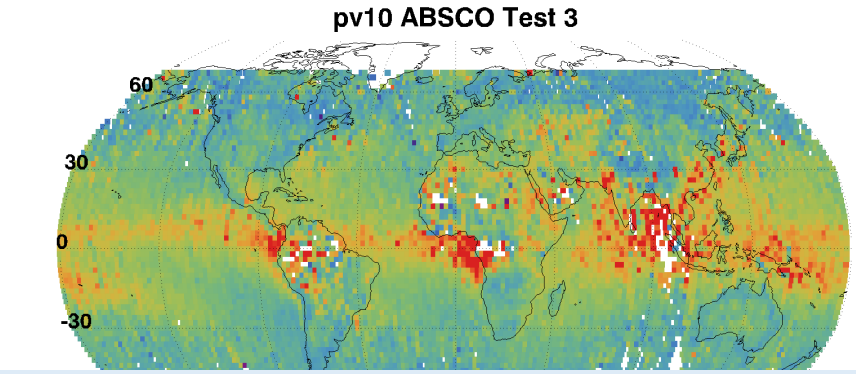
Line database swap had some small impact on PSUR

Impact on retrieved XCO_2

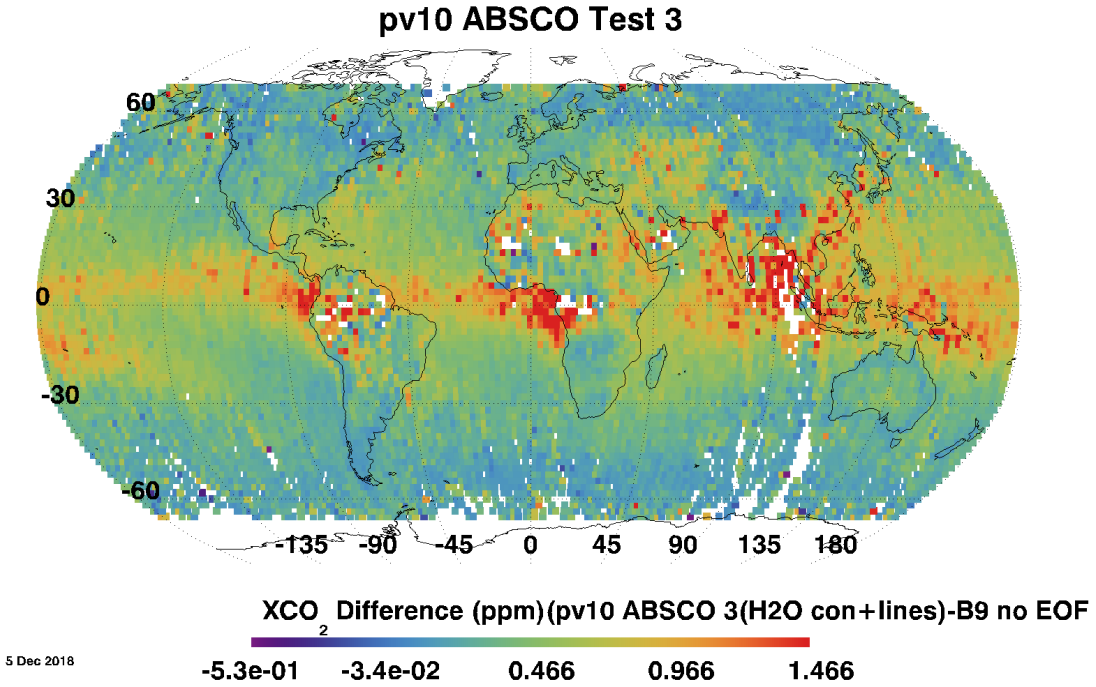


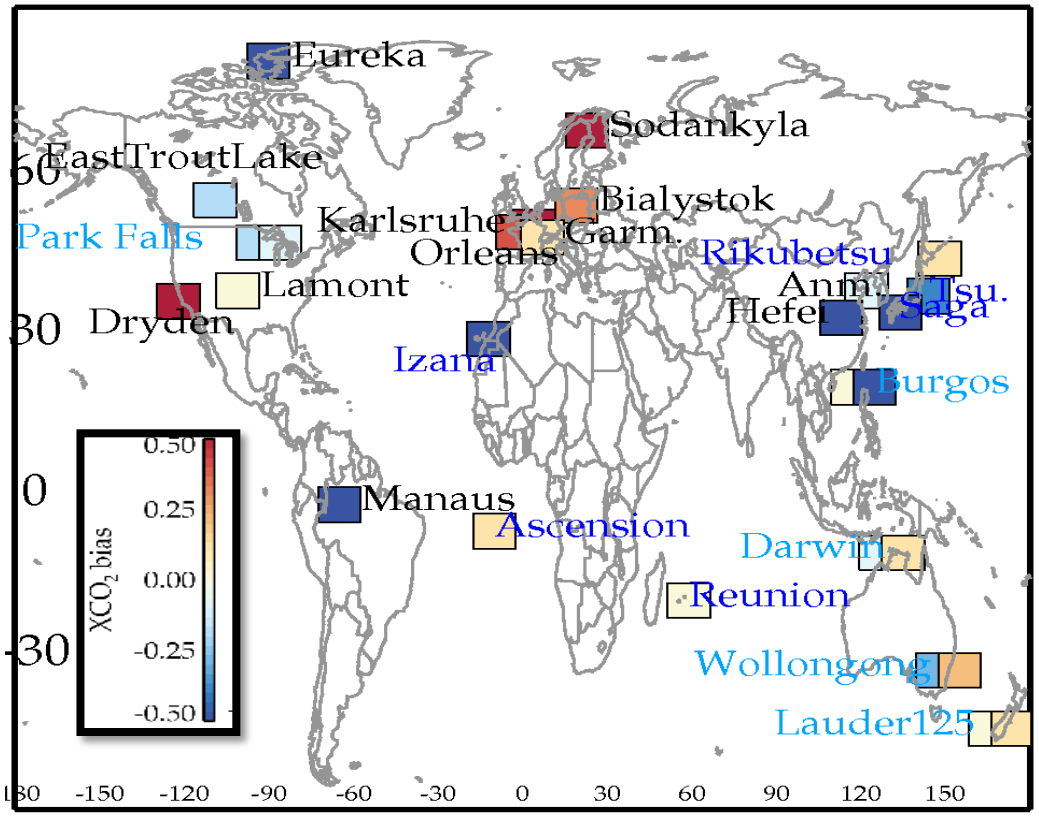
Update adopted for ABSCO v.1

Continuum update: XCO2 impact strongly correlated with PSUR



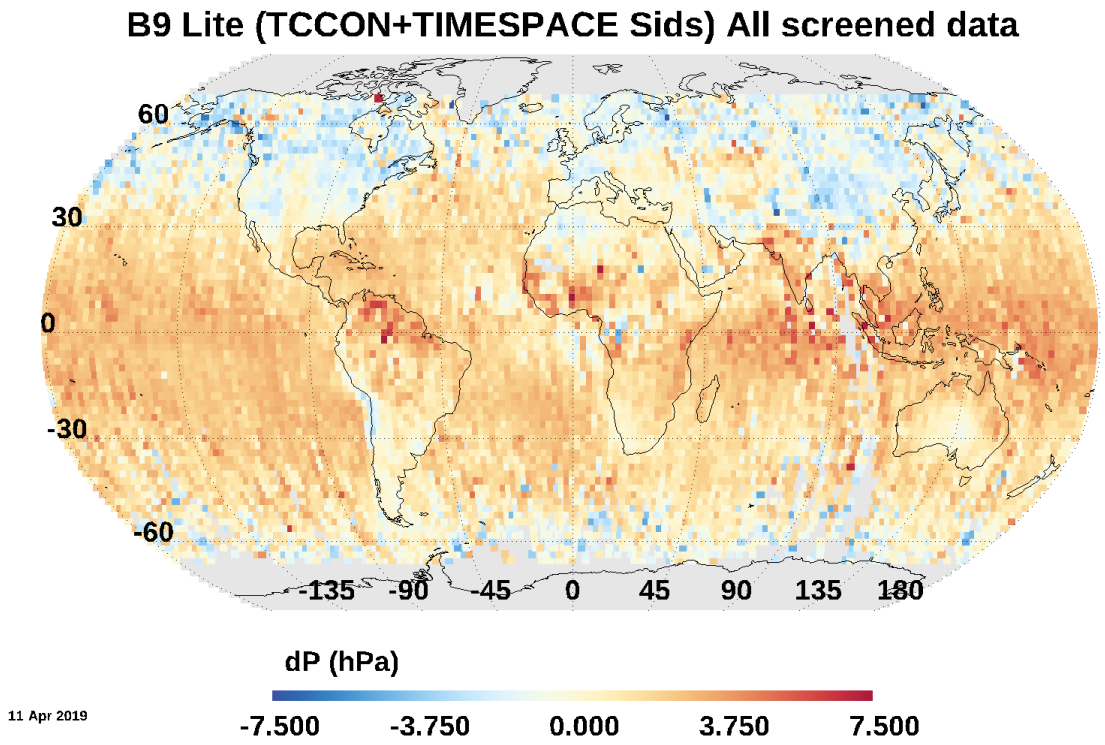
Line database impacts XCO2 separately from PSUR

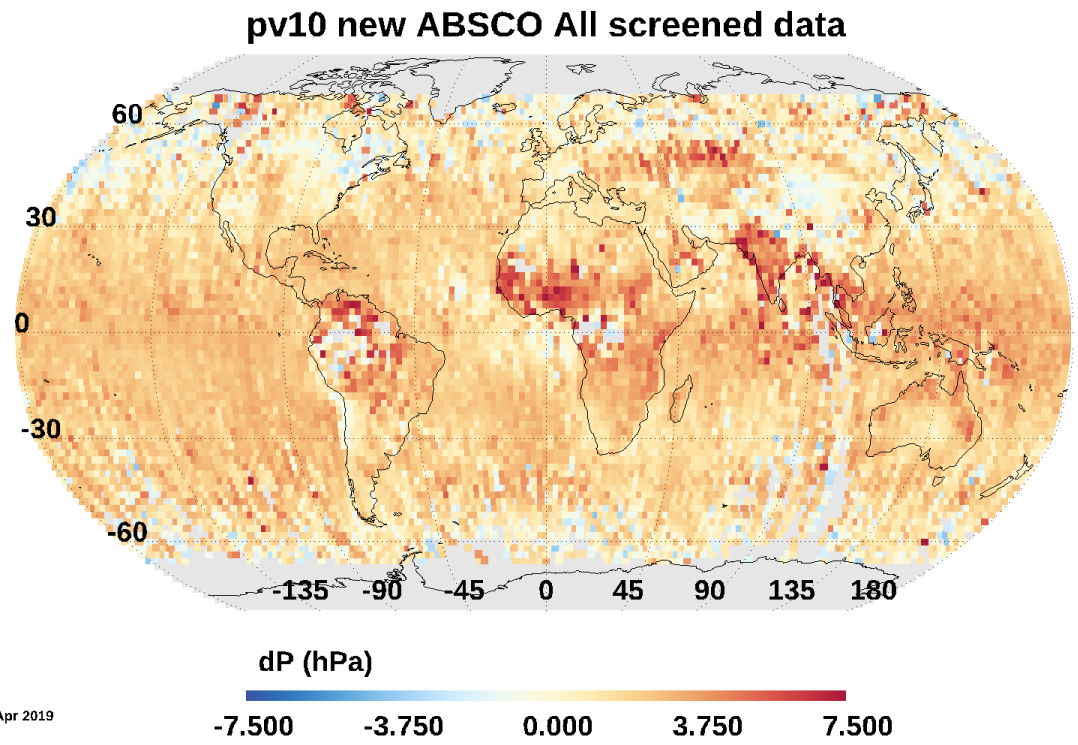




Kulawik et al., in prep

O2 A-band: testing with EOFs



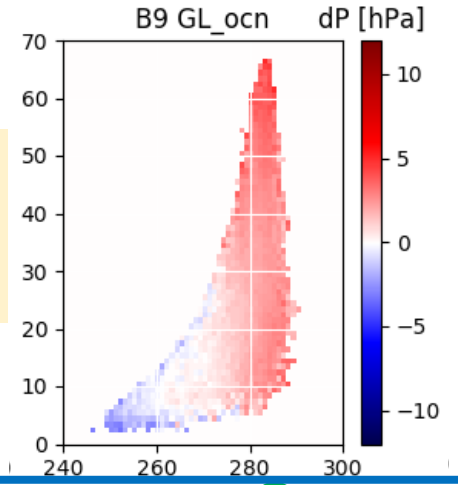


- Not yet done: with EOFs, but with cleanest test set

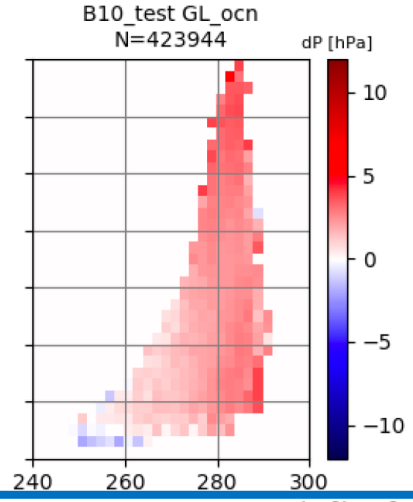
Plots from Aronne Merrelli: Column water, T at 700 mbar

Ocean glint cases only

Top row has EOFs included

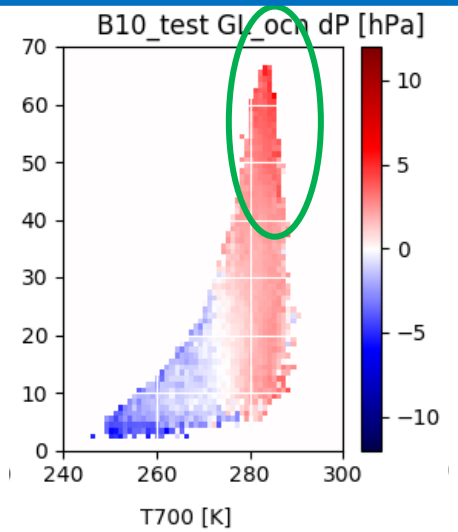


Note: Plots with EOFs included are based on different test datasets

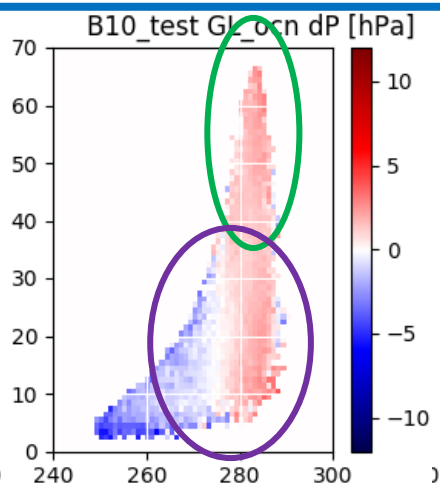


Lower row: Tests

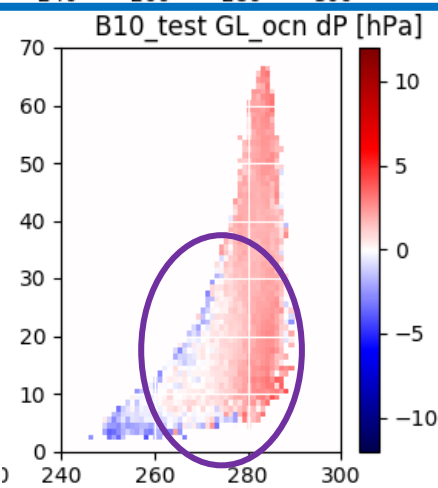
Test have no EOFs



No-EOF baseline



H2O continuum update

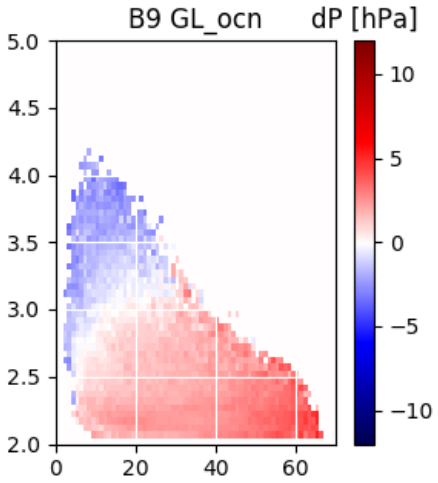


O2 update

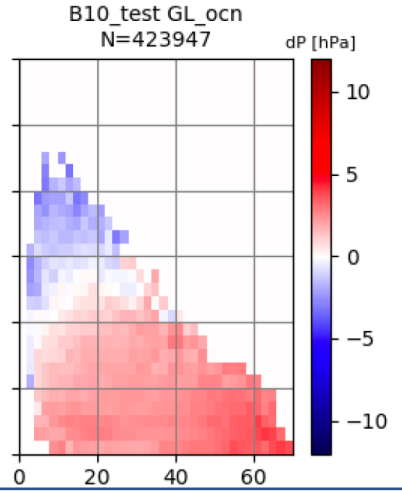
Plots from Aronne Merrelli: Airmass, Column water

Ocean glint cases only

Top row has EOFs included

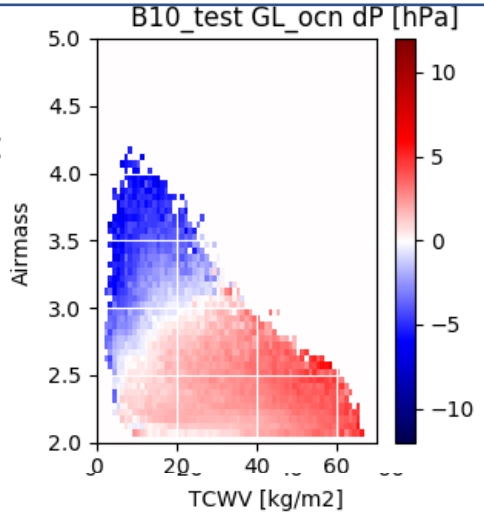


Note: Plots with EOFs included are based on different test datasets

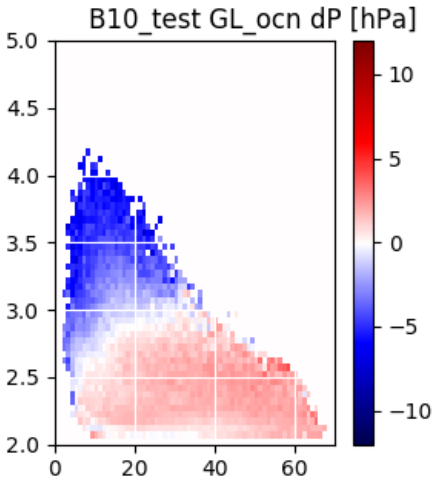


Lower row: Tests

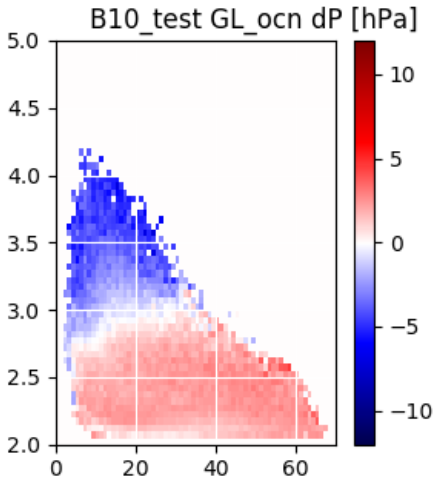
Tests have no EOFs



No-EOF baseline

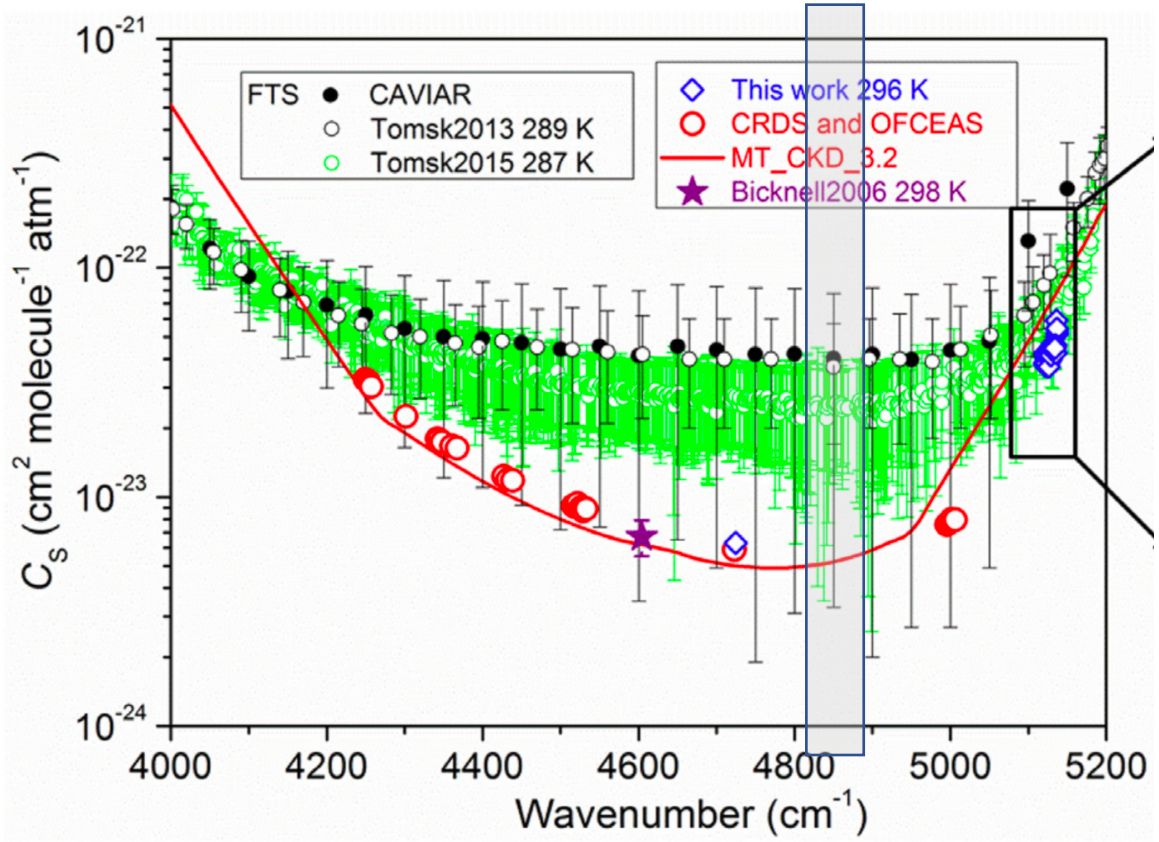


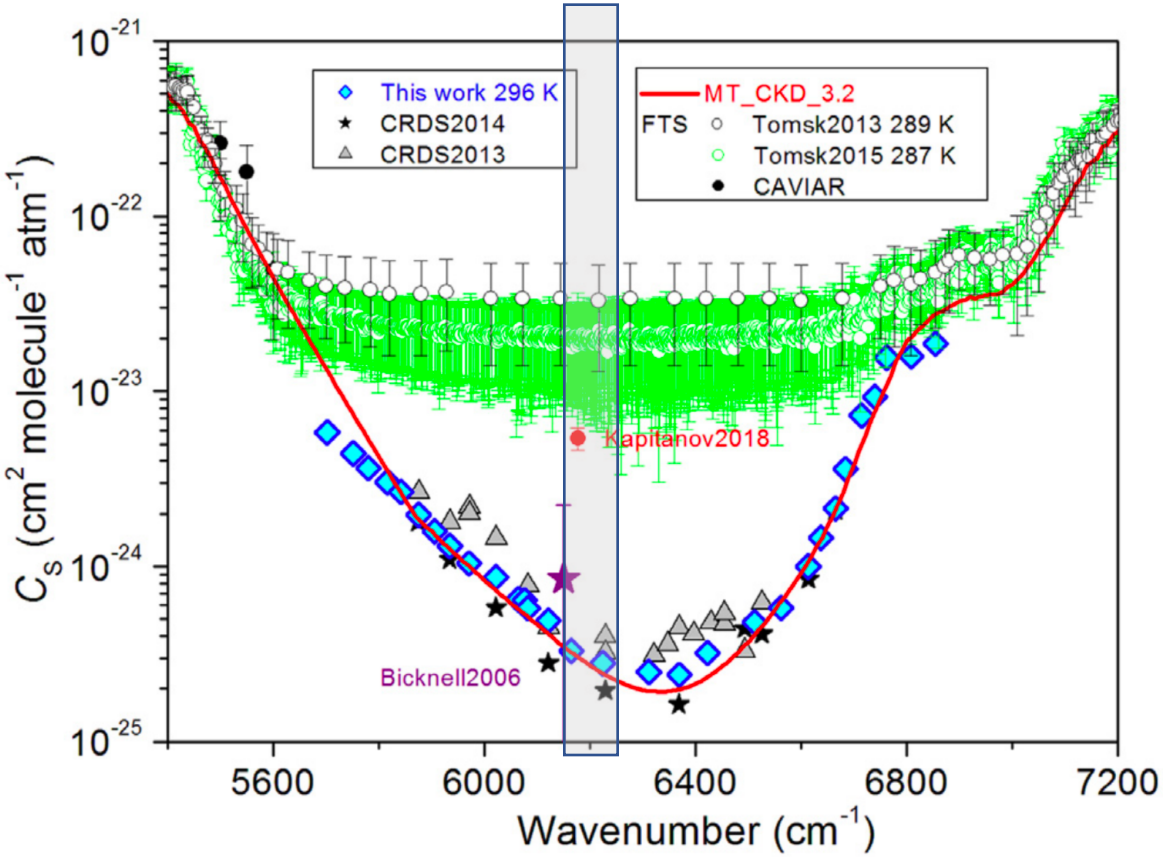
H2O continuum update



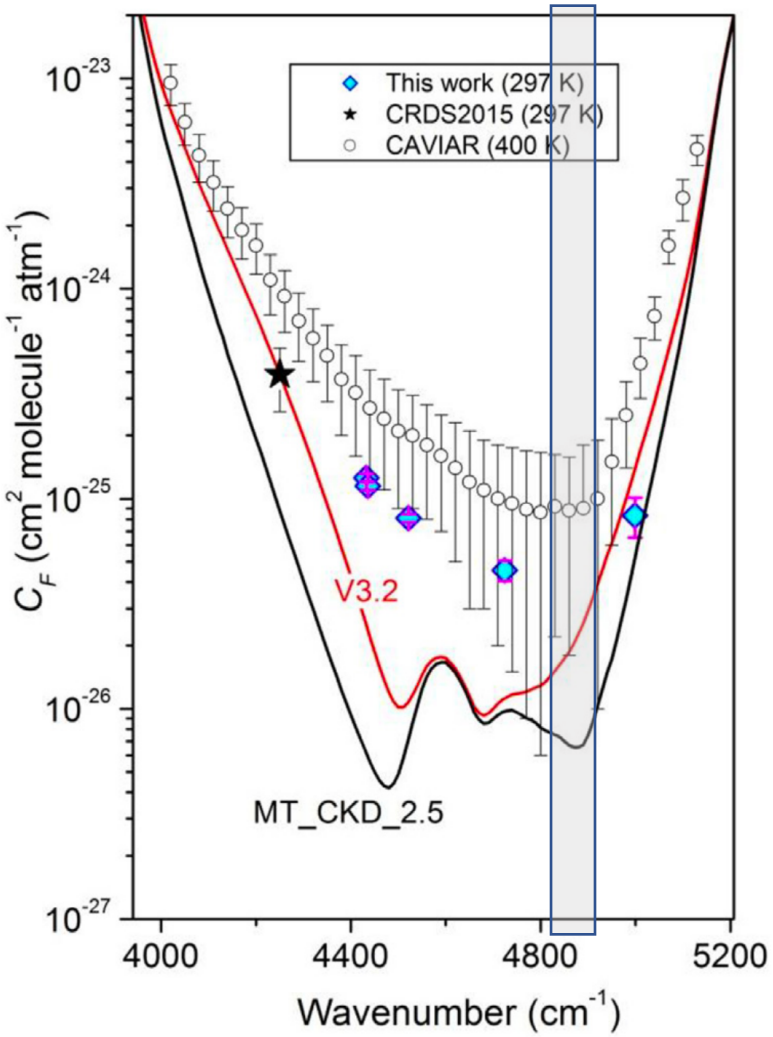
O2 update

Vasilchenko et al. [2019]: Self-broadened





Vasilchenko et al. [2019]: Foreign-broadened



New CRDS measurements suggest need for an increase in foreign continuum (relative to MT_CKD)

Some slope in the difference

Factor of 2-3 at low wavenumber end of SCO2 band